Soot Formation Modeling of n-dodecane and Diesel Sprays under Engine-Like Conditions - DTU Orbit (08/11/2017)

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This work concerns the modelling of soot formation process in diesel spray combustion under engine-like conditions. The key aim is to investigate the soot formation characteristics at different ambient temperatures. Prior to simulating the diesel combustion, numerical models including a revised multi-step soot model is validated by comparing to the experimental data of n-dodecane fuel in which the associated chemistry is better understood. In the diesel spray simulations, a single component n-heptane mechanism and the multi-component Diesel Oil Surrogate (DOS) model are adopted. A newly developed C16-based model which comprises skeletal mechanisms of n-hexadecane, heptamethylnonane, cyclohexane and toluene is also implemented. Comparisons of the results show that the simulated liftoff lengths are reasonably well-matched to the experimental measurement, where the relative differences are retained to below 18%. Only that predicted by the DOS model in the 900 K case is overestimated by approximately 28%. The experimental maximum soot volume fraction (SVF) rises by approximately 7.0 fold as the ambient temperature is raised from 900 K to 1000 K. The ratio calculated by chemical mechanisms without toluene chemistry is approximately two-fold. Improvement is observed when toluene chemistry is considered, producing ratios of greater than 3.7. This can be attributed to the higher amount of soot precursor and surface growth species formed through the toluene oxidation pathways in the 1000 K case. A surrogate model that considers the kinetics of aromatic compounds is hence more promising to improve the prediction of local SVF which is significant to soot radiation modelling.

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